

Kohn-Luttinger instability of the t - t' Hubbard model in two dimensions: variational approach

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An effective Hamiltonian for the Kohn-Luttinger superconductor is constructed and solved in the BCS approximation. The method is applied to the t - t' Hubbard model in two dimensions with the following results: (i) The superconducting phase diagram at half filling is shown to provide a weak-coupling analog of the recently proposed spin liquid state in the J_1 - J_2 Heisenberg model. (ii) In the parameter region relevant for the cuprates we have found a nontrivial energy dependence of the gap function in the dominant d -wave pairing sector. The hot spot effect in the angular dependence of the superconducting gap is shown to be quite weak.

I. INTRODUCTION

In a seminal paper, Kohn and Luttinger¹ (KL) presented a perturbative argument showing that the generic ground state of a Fermi liquid at weak coupling is superconducting, even if the bare electron-electron interaction is not attractive in the Cooper channel in any angular momentum sector. Recently, this result has been re-derived utilizing various versions of the renormalization group method.^{2,3,4}

However, no attempt has been made so far to construct a variational wavefunction for a KL superconductor, which could be (at least in principle) tested in a direct numerical simulation. The purpose of this paper is to construct such a wavefunction for the repulsive Hubbard model in the limit of weak coupling $U \ll W$, where U is the local repulsive interaction and W is the electron bandwidth. Our strategy follows quite closely the canonical transformation approach to the electron-phonon problem introduced by Fröhlich⁵ and sketched in the Appendix. In some sense it is also similar to the customary analysis of the Hubbard model close to half filling in the limit of strong coupling $U \gg W$. Namely, in the latter case a canonical transformation can be found^{6,7} which transforms the purely repulsive Hubbard model to the so-called t - J model which explicitly contains an attractive interaction (of the order $J \sim W^2/U$) favoring the formation of singlet superconductivity. Unfortunately, the t - J model contains a constraint on the local number of electrons and as such is very difficult to study. Here, on the other hand, we construct a canonical transformation which eliminates the scattering of quasiparticles to first order in U/W and generates a weak-coupling model with an attractive interaction of the order U^2/W .

The outline of the paper is as follows. The construction of the effective model is described in Section II and our method is applied to the two-dimensional t - t' Hubbard model in Section III.

II. EFFECTIVE HAMILTONIAN

We consider the Hubbard model on a square lattice with periodic boundary conditions and $L = l \times l$ sites,

described by the Hamiltonian $H = H_0 + H_1 + H_2$, where $H_0 = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k},\sigma}$ is the kinetic energy operator and the interaction term has been split into two parts:

$$H_1 = \frac{U}{L} \left(\frac{N^2}{4} - \mathbf{S}^2 \right) + \frac{U}{L} \sum_{\mathbf{k},\mathbf{p}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow}, \quad (1)$$

$$H_2 = \frac{U}{L} \sum'_{\{\mathbf{k}\}} c_{\mathbf{k}_3\uparrow}^\dagger c_{\mathbf{k}_1\uparrow} c_{\mathbf{k}_4\downarrow}^\dagger c_{\mathbf{k}_2\downarrow} \delta_{\mathbf{k}_1+\mathbf{k}_2, \mathbf{k}_3+\mathbf{k}_4}, \quad (2)$$

where $N = N_\uparrow + N_\downarrow$ and \mathbf{S} are the total electron number and the total spin, respectively. Terms which are not extensive in the thermodynamic limit $L \rightarrow \infty$ have been neglected. H_2 is the generic interaction term which scatters electrons from $\mathbf{k}_1 \uparrow$ to $\mathbf{k}_3 \uparrow$ and from $\mathbf{k}_2 \downarrow$ to $\mathbf{k}_4 \downarrow$. The prime on the summation means that terms with $\mathbf{k}_1 = \mathbf{k}_3$ (forward scattering channel), $\mathbf{k}_1 = \mathbf{k}_4$ (exchange channel), and $\mathbf{k}_1 + \mathbf{k}_2 = 0$ (Cooper channel) are excluded from H_2 and are singled out into H_1 . The operator $H_0 + H_1$ can be thought of as a reduced BCS Hamiltonian of a Landau Fermi liquid, while H_2 contains the scattering processes leading to a finite lifetime of the Landau quasiparticles.

Now we look for a canonical transformation from the bare electrons to the dressed ones, $\tilde{H} = e^{iS} H e^{-iS}$, such that the scattering of the quasiparticles vanishes to first order in U . This happens if $H_2 + i[S, H_0] = 0$ in which case we can write $\tilde{H} = H_0 + H_1 + i[S, H_1] + i[S, H_2]/2$, where terms of order $O(U^3)$ have been neglected. Making use of the identity

$$[c_P^\dagger c_Q, c_R^\dagger c_S] = \delta_{QR} c_P^\dagger c_S - \delta_{PS} c_R^\dagger c_Q \quad (3)$$

where the indices P, Q, R, S include also the spin label, one verifies readily that

$$S = \frac{iU}{L} \sum'_{\{\mathbf{k}\}} \frac{\delta_{\mathbf{k}_1+\mathbf{k}_2, \mathbf{k}_3+\mathbf{k}_4}}{\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_3} - \varepsilon_{\mathbf{k}_4}} c_{\mathbf{k}_3\uparrow}^\dagger c_{\mathbf{k}_1\uparrow} c_{\mathbf{k}_4\downarrow}^\dagger c_{\mathbf{k}_2\downarrow} \quad (4)$$

is the Hermitian generator we are looking for. Note that the forward, exchange, and Cooper channel processes do not contribute to S . In order to calculate the commutators $[S, H_1]$ and $[S, H_2]$ we first note that the operators

$A = c_{3\uparrow}^\dagger c_{1\uparrow}$ and $B = c_{\gamma\uparrow}^\dagger c_{\alpha\uparrow}$ commute with the operators $X = c_{4\downarrow}^\dagger c_{2\downarrow}$ and $Y = c_{\delta\downarrow}^\dagger c_{\beta\downarrow}$ and therefore

$$[AX, BY] = [A, B]XY + BA[X, Y]. \quad (5)$$

Combining Eqs. (3,5) we thus find the identity

$$[c_{3\uparrow}^\dagger c_{1\uparrow} c_{4\downarrow}^\dagger c_{2\downarrow}, c_{\gamma\uparrow}^\dagger c_{\alpha\uparrow} c_{\delta\downarrow}^\dagger c_{\beta\downarrow}] = (\delta_{1\gamma} c_{3\uparrow}^\dagger c_{\alpha\uparrow} - \delta_{3\alpha} c_{\gamma\uparrow}^\dagger c_{1\uparrow}) c_{4\downarrow}^\dagger c_{2\downarrow} c_{\delta\downarrow}^\dagger c_{\beta\downarrow} + (\delta_{2\delta} c_{4\downarrow}^\dagger c_{\beta\downarrow} - \delta_{4\beta} c_{\delta\downarrow}^\dagger c_{2\downarrow}) c_{\gamma\uparrow}^\dagger c_{\alpha\uparrow} c_{3\uparrow}^\dagger c_{1\uparrow},$$

making use of which one can straightforwardly calculate the effective Hamiltonian \tilde{H} . The result is fairly involved, including also three-body forces among the electrons. Nevertheless, the expectation value $E = \langle \tilde{\psi} | \tilde{H} | \tilde{\psi} \rangle$ in a BCS state $|\tilde{\psi}\rangle = \Pi_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger) |0\rangle$ takes a simple and physically transparent form,

$$E = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} f_{\mathbf{k}\sigma} + \frac{U}{L} \frac{N^2}{4} + \frac{1}{L} \sum_{\mathbf{k}, \mathbf{p}} V_{\mathbf{k}\mathbf{p}} b_{\mathbf{k}}^* b_{\mathbf{p}} + \frac{U^2}{L^2} \sum_{\{\mathbf{k}\}}' \frac{f_{\mathbf{k}_1} f_{\mathbf{k}_2} (1 - f_{\mathbf{k}_3}) (1 - f_{\mathbf{k}_4})}{\varepsilon_{\mathbf{k}_1} + \varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_3} - \varepsilon_{\mathbf{k}_4}} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_4}, \quad (6)$$

where we have introduced a momentum-resolved BCS order parameter $b_{\mathbf{p}} = \langle \tilde{\psi} | c_{-\mathbf{p}\downarrow} c_{\mathbf{p}\uparrow} | \tilde{\psi} \rangle$ and we assumed $\langle \tilde{\psi} | \mathbf{S}^2 | \tilde{\psi} \rangle = 0$. In the Cooper channel the effective interaction reads $V_{\mathbf{k}\mathbf{p}} = U + U^2 \chi_1(\mathbf{k} + \mathbf{p}, \varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{k}})$, where $\chi_1(\mathbf{q}, \omega)$ is the real part of the particle-hole susceptibility $\chi(\mathbf{q}, \omega) = L^{-1} \sum_{\mathbf{K}} (f_{\mathbf{K}} - f_{\mathbf{K}+\mathbf{q}}) / (\varepsilon_{\mathbf{K}+\mathbf{q}} - \varepsilon_{\mathbf{K}} - \omega - i0)$. The physical content of the KL argument is that the effective interaction between the dressed electrons can be attractive in the Cooper channel in some angular momentum sector. If this is the case, then the energy $E = \langle \tilde{\psi} | e^{iS} H e^{-iS} | \tilde{\psi} \rangle$ is minimized by nonvanishing $b_{\mathbf{p}}$ and the wavefunction $|\psi\rangle = e^{-iS} |\tilde{\psi}\rangle$ provides a variational ansatz for the KL superconductor.

Before proceeding we would like to point out that our variational approach bears some similarity to a very recent formulation of the flow equation method.⁸ The comparison of both methods is left for future.

III. BCS VARIATIONAL SOLUTION OF THE EFFECTIVE HAMILTONIAN

We wish to apply the above formalism to the study of the t - t' Hubbard model in two dimensions whose single particle dispersion is $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y$, where we have set the lattice constant $a = 1$. The superconducting phase diagram of the weak-coupling t - t' Hubbard model has been studied previously by considering the effective KL interaction $V_{\mathbf{k}\mathbf{p}}^{KL} = U + U^2 \chi_1(\mathbf{k} + \mathbf{p}, 0)$ with both \mathbf{k} and \mathbf{p} lying at the Fermi surface.⁹ Roughly speaking, such an approach provides us with the coupling constant g , but not with the prefactor Ω in the BCS formula for the transition temperature, $T_c = \Omega \exp(-1/g)$.

In what follows we perform the standard BCS minimization of an effective free energy whose $T = 0$ limit reduces to the variational energy Eq. (6). We assume that

the interaction U is sufficiently weak so that no particle-hole instabilities can develop. (In particular, this means that we can't study systems close to the van Hove filling.) Concentrating on lowest order effects in U/W , we neglect the last term in Eq. (6) which represents the standard second-order perturbation theory effects, and treat it as an additive constant. A more detailed study of Eq. (6) taking into account also the last term is postponed to future publications. Moreover, since we expect that $T_c \ll t$, we make use of the $T = 0$ Fermi functions in the calculation of the particle-hole susceptibility $\chi(\mathbf{q}, \omega)$.

A standard BCS calculation leads to the self-consistent equation for the gap function $\Delta_{\mathbf{k}} = L^{-1} \sum_{\mathbf{p}} V_{\mathbf{k}\mathbf{p}} b_{\mathbf{p}}$,

$$\Delta_{\mathbf{k}} = -\frac{1}{L} \sum_{\mathbf{p}} V_{\mathbf{k}\mathbf{p}} \Delta_{\mathbf{p}} \frac{\tanh(E_{\mathbf{p}}/2T)}{2E_{\mathbf{p}}}, \quad (7)$$

where $E_{\mathbf{p}} = (\xi_{\mathbf{p}}^2 + \Delta_{\mathbf{p}}^2)^{1/2}$, $\xi_{\mathbf{p}} = \varepsilon_{\mathbf{p}} - \mu$, and μ is the chemical potential.

For temperatures infinitesimally below the mean field transition temperature, the gap equation can be linearized with respect to $\Delta_{\mathbf{p}}$ and can be written as $D_{\mathbf{k}} = \sum_{\mathbf{p}} I_{\mathbf{k}\mathbf{p}}(T) D_{\mathbf{p}}$, where $D_{\mathbf{k}} = \Delta_{\mathbf{k}} \phi_{\mathbf{k}} T^{-1/2}$ is a dimensionless gap function, $\phi_{\mathbf{k}} = [\tanh(\xi_{\mathbf{k}}/2T)/2\xi_{\mathbf{k}}]^{1/2}$, and $I_{\mathbf{k}\mathbf{p}}(T) = -L^{-1} V_{\mathbf{k}\mathbf{p}} \phi_{\mathbf{k}} \phi_{\mathbf{p}}$ is a real symmetric matrix corresponding to a dimensionless pair scattering function. At high temperatures $I_{\mathbf{k}\mathbf{p}}(T) \propto T^{-1}$ and the gap equation does not have solutions. With decreasing T the maximal eigenvalue λ of $I_{\mathbf{k}\mathbf{p}}(T)$ grows and the mean field transition temperature T_c can be calculated from the condition $\lambda(T_c) = 1$.

We have studied the eigenvalues of $I_{\mathbf{k}\mathbf{p}}(T)$ numerically. In order to minimize the cost of the calculation, the matrix $I_{\mathbf{k}\mathbf{p}}$ was calculated on a special lattice, see Fig. 1. The lattice consists of a sequence $i = 1, 2, \dots, n$ of n regular $l_i \times l_i$ grids, which become progressively more dense as the distance to the Fermi level diminishes, $l_{i+1} = 2l_i$. The borders between the subsequent

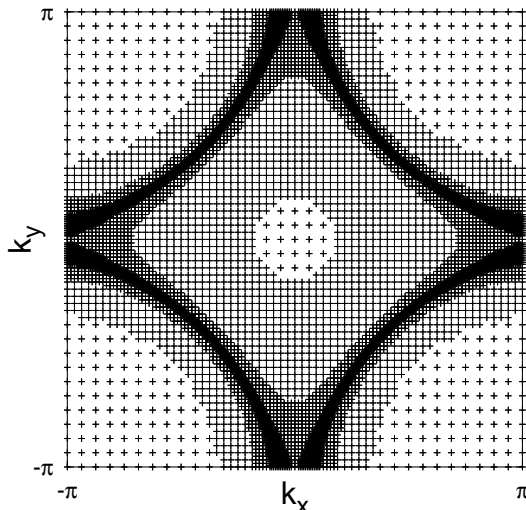


FIG. 1: An example of the special set of \mathbf{k} points in the first Brillouin zone for $t'/t = 0.3$ and $\rho = 0.8$. Under approaching the Fermi energy, the grid changes in each level (there are 4 levels in total) from 32×32 to 256×256 .

levels are constructed as follows: Let the maximum and minimum band energies be ξ_{\max} and ξ_{\min} and let $\xi_0 = \max(\xi_{\max}, |\xi_{\min}|)$. We construct a sequence of energies $\xi_i = q^i \xi_0$ with a quotient $q < 1$. For $i < n$, the i -th level grid $l_i \times l_i$ is realized for all \mathbf{k} points satisfying $\xi_i < |\xi_{\mathbf{k}}| < \xi_{i-1}$, whereas the n -th grid applies for $|\xi_{\mathbf{k}}| < \xi_{n-1}$. The lattice is characterized by three parameters: q , l_1 , and the number of levels n . In what follows we always take $q = 4^{-1}$ and $l_1 = 32$, and instead of the number of levels we describe the lattice by specifying the finest \mathbf{k} -point grid $l_n \times l_n$.

The susceptibility $\chi(\mathbf{q}, \omega)$ was calculated on usual lattices $l_n \times l_n$ by a straightforward modification of the method described in Ref. 10 which makes use of the fast Fourier transform algorithm. We have used $4l_n$ time points and the Nyquist frequency was chosen to be $8W$.

The matrix $I_{\mathbf{k}\mathbf{p}}$ was diagonalized by the modified Lanczos method.¹¹ The initial vector was generated randomly in one octant (quadrant) of the Brillouin zone and subsequently continued to the whole zone so as to transform according to the one-dimensional s , d , d_{xy} and g (two-dimensional p) irreducible representations of the point group of the square.¹²

As an illustrative example, the temperature dependence of the maximal eigenvalue in the d_{xy} sector for $t'/t = 0.78$ and electron density $\rho = 1$ is shown in Fig. 2 for various $l_n \times l_n$. Several points are worth mentioning. For a finite lattice size l_n , the divergence of the particle-particle susceptibility is cut off at temperatures $T^* \sim v_F/l_n$, and therefore $\lambda(T)$ saturates at low temperatures $T \ll T^*$. Thus, even making use of a moderate interaction strength¹³ $U = W/2$ (this value of U is used in most numerical examples) the largest eigenvalue λ of $I_{\mathbf{k}\mathbf{p}}$ is typically less than unity down to the lowest tem-

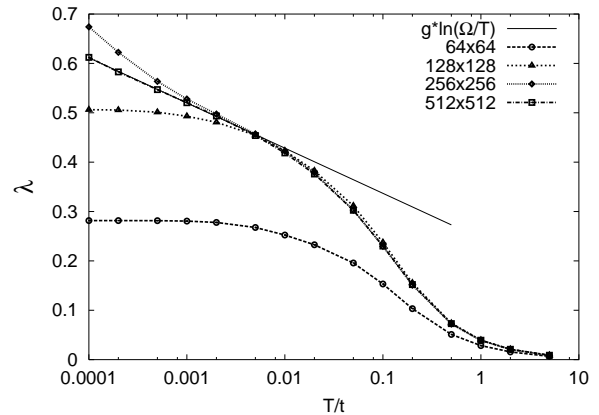


FIG. 2: The temperature dependence of the largest eigenvalue in the d_{xy} -wave sector for $U = W/2$, $t'/t = 0.78$, and $\rho = 1$. The line is a fit to $\lambda(T) = g \log(\Omega/T)$. The fitting parameters $g = 0.04$ and $\Omega/t = 480$ imply $T_c/t = 6.05 \times 10^{-9}$.

peratures. Therefore we can't determine T_c directly from $\lambda(T_c) = 1$. Instead, the T -dependence of the eigenvalue is fitted in the low temperature limit by a BCS-like expression $\lambda(T) = g \log(\Omega/T)$ and afterwards T_c is calculated from $T_c = \Omega \exp(-1/g)$. This procedure is shown explicitly in Fig. 2. It should be pointed out that usually we can determine the transition temperature with a reasonable degree of confidence only if $T_c/t > 10^{-6}$. In this sense the parameter values used in Fig. 2 are somewhat special.

Let us also stress that the large value of Ω estimated from Fig. 2 should not be interpreted as a large pairing energy scale. This is evident from an equivalent but physically more meaningful expression $\lambda(T) = \lambda(T_0) + g \log(T_0/T)$ which makes explicit use of the pairing energy T_0 (its value is arbitrary, but can be estimated from the maximal temperature where the logarithmic scaling of λ applies, $T_0 \sim 0.005t$ in our example). The large value of $\Omega = T_0 \exp[\lambda(T_0)/g]$ is a consequence of the large $\lambda(T_0)$, which in turn measures the contribution of the high energy processes to λ .

A. Half-filled t - t' Hubbard model

Now let us apply the abovementioned method to the study of the superconducting phase diagram of the t - t' Hubbard model at half filling ($\rho = 1$). In the strong-coupling limit $U \gg W$, this would correspond to the Heisenberg model $H = J_1 \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}} + J_2 \sum_{\langle\langle \mathbf{i}, \mathbf{j} \rangle\rangle} \mathbf{S}_{\mathbf{i}} \cdot \mathbf{S}_{\mathbf{j}}$, where $\langle \mathbf{i}, \mathbf{j} \rangle$ and $\langle\langle \mathbf{i}, \mathbf{j} \rangle\rangle$ are pairs of nearest neighbor and next-nearest neighbor sites, respectively, $J_1 = 4t^2/U$, and $J_2 = 4(t')^2/U$. There is general consensus that, due to frustration, for $0.4 < J_2/J_1 < 0.6$ the Heisenberg model does not exhibit the Néel order (see, e.g. Ref. 14 and references therein). The nature of the emergent state has been discussed intensively, but very recently it has been shown¹⁴ that a projected BCS wavefunction with a

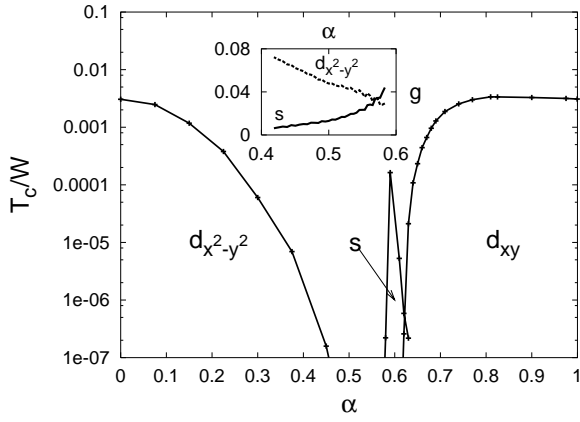


FIG. 3: Superconducting phase diagram for the half filled Hubbard model at $U = W/2$. The inset shows the coupling constant g in the d and s sectors, calculated according to Ref. 9 in the region where T_c is not directly accessible.

mixed d and d_{xy} symmetry provides a very good approximation for the J_1 - J_2 model with J_2/J_1 close to $1/2$.

In this paper we look for a weak-coupling analogue of the phase proposed by Capriotti *et al.*¹⁴ To this end, in Fig. 3 we plot T_c in the d -wave and d_{xy} -wave sectors as a function of $\alpha = 2t'/(t + 2t')$ for $U = W/2$ and $\rho = 1$. The dominant pairing instability is seen to change from the d -wave at small t'/t to the d_{xy} symmetry at large t'/t , since the susceptibility $\chi(\mathbf{q}, 0)$ peaks at (π, π) and $(\pi, 0)$ in these two limits. Surprisingly, in the region corresponding to $J_2/J_1 \approx 1/2$, namely $t'/t \approx 2^{-1/2}$ or $\alpha \approx 0.59$, we find that neither d nor d_{xy} -wave pairing instabilities are dominant, and a small island of s -wave pairing is realized. For $\alpha \in [0.45, 0.57]$ the transition temperatures are too low to be accessible by the present method. Therefore we show in Fig. 3 the coupling constant g in the (dominant) d and s -wave symmetry sectors calculated according to Ref. 9. From the qualitative agreement of these two different methods we conclude that in the vicinity of $\alpha \sim 0.55$ the pairing symmetry changes from d to s -wave.

We expect that for $\alpha \approx 0.59$, upon increase of the interaction strength there is presumably a true Mott-Hubbard superconductor-insulator transition at some critical value of U . We hypothesize that before this happens, with increasing U the d and d_{xy} phases grow at the expense of the s phase, until at some stage the s phase disappears from the phase diagram. On the other hand, underneath the crossing point of the d -wave and d_{xy} -wave T_c 's, we expect a region with mixed $d + id_{xy}$ pairing. Such mixed-symmetry pairing can be justified by a simple model calculation for a two dimensional isotropic system with a separable interaction $V(\phi, \phi') = V_1(\phi, \phi') + V_2(\phi, \phi')$ in the Cooper channel. Here $V_1(\phi, \phi') \propto \cos 2\phi \cos 2\phi'$ with coupling constant g_1 and cutoff ω_1 leads to d -wave pairing and $V_2(\phi, \phi') \propto \sin 2\phi \sin 2\phi'$ with coupling constant g_2 and cutoff ω_2 yields d_{xy} -wave pairing. For simplicity we further assume that by changing a control parameter (t'/t in our case), only the coupling constant g_2 changes.

Then, if we denote that value of g_2 for which the T_c crossing happens as g_2 , it can be shown readily that a mixed $d + id_{xy}$ pairing state is in fact stabilized at zero temperature in a finite window of the control parameter for which $g_{20}^{-1} - 1/2 < g_2^{-1} < g_{20}^{-1} + 1/2$. Note that in the weak-coupling limit this window is quite narrow.

Before proceeding we should mention that the concept of mixed-symmetry superconductivity has been introduced previously in the context of strong coupling models, for the t - J model by Kotliar¹⁵ and for the t - t' - J_1 - J_2 model in a recent paper by Sachdev.¹⁶ Our discussion shows that (as pointed out already in Ref.9), mixed-symmetry superconductivity is in fact a generic consequence of phase diagrams like the one shown in Fig. 3, where superconducting states of different symmetry cross.

B. d -wave region of the t - t' Hubbard model

As another application of the present formalism, in the rest of this paper we concentrate on the d -wave region of the superconducting phase diagram of the t - t' Hubbard model⁹ which is relevant to the cuprates. Close to the van Hove density, superconductivity competes with the SDW state^{4,9,18} and the question whether one of these two states or even more exotic states¹⁷ wins is still open. Here we focus on a different question, namely that of the full \mathbf{k} -dependence of the superconducting gap $\Delta_{\mathbf{k}}$ away from the van Hove density. Fig. 4 shows the self-consistent solution $\Delta_{\mathbf{k}}$ of Eq. (7) for $t'/t = 0.3$, $\rho = 0.8$, and $T = 0$. The maximal gap on the Fermi surface $\Delta_{\max} = 0.0023t$ and the critical temperature $T_c = 0.0013t$ imply $\Delta_{\max}/T_c \approx 1.8$.

The overall shape of $\Delta_{\mathbf{k}}$ is well described by the simplest formula consistent with d -wave symmetry, $\Delta_{\mathbf{k}} \propto \cos k_x - \cos k_y$. Nevertheless, fine structure on top of this overall shape is clearly visible. This is shown more quantitatively in Fig. 5, where $\Delta_{\mathbf{k}}$ is plotted along two $k_y = \text{const}$ cuts of the Brillouin zone. A nontrivial structure is seen to develop in the direction perpendicular to the Fermi surface which is analogous to the strong-coupling effects in conventional superconductors.

It is well known that in the case of phonon mediated superconductivity the energy dependence of $\Delta_{\mathbf{k}}$ leads to a structure in the density of states. In the Appendix we have shown that our method is capable to describe such effects. Therefore we have looked for features in the density of states caused by the structure in $\Delta_{\mathbf{k}}$ in our purely electronic model as well. The electron spectral function $A(\mathbf{k}, \omega)$ and the density of states $N(\omega)$ have been calculated from

$$A(\mathbf{k}, \omega) = u_{\mathbf{k}}^2 \delta(\omega - E_{\mathbf{k}}) + v_{\mathbf{k}}^2 \delta(\omega + E_{\mathbf{k}}), \quad (8)$$

$$N(\omega) = L^{-1} \sum_{\mathbf{k}} A(\mathbf{k}, \omega), \quad (9)$$

where $u_{\mathbf{k}}^2, v_{\mathbf{k}}^2 = 2^{-1}(1 \pm \xi_{\mathbf{k}}/E_{\mathbf{k}})$. Fig. 6 shows that at weak coupling (e.g. for $U = W/2$ when $\Delta, T_c \ll t$) no struc-

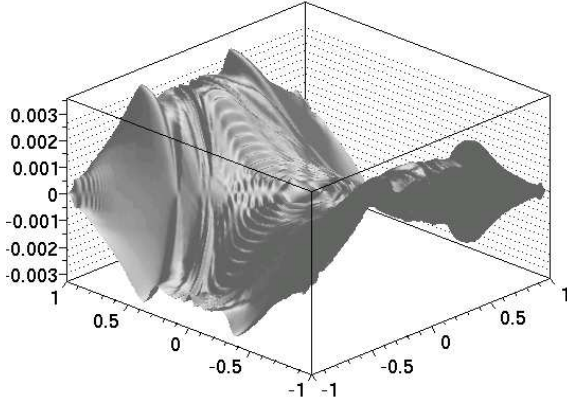


FIG. 4: The self-consistent solution $\Delta_{\mathbf{k}}$ in the d -wave sector (in units of t) as a function of momentum in the first Brillouin zone for $T = 0$, $U = W/2$, $t'/t = 0.3$, and $\rho = 0.8$. Calculated on a full lattice $L = 256 \times 256$. The momenta k_x and k_y are measured in units of π .

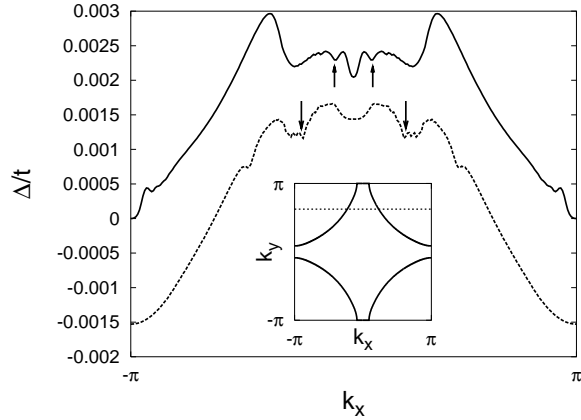


FIG. 5: Cuts of the data in Fig. 4 along the lines $k_y = \pi$ (top) and $k_y = 5\pi/8$ (bottom). The crossing points of the $k_y = \text{const}$ lines with the Fermi surface are indicated by arrows. The inset shows the Fermi surface for $t'/t = 0.3$ and $\rho = 0.8$, and the location of the cuts.

tures associated with the energy dependence of $\Delta_{\mathbf{k}}$ can be observed. This is because features in the energy dependence of $\Delta_{\mathbf{k}}$ can be visible also in the density of states only if they appear in a \mathbf{k} -point for which the single-particle energy $\xi_{\mathbf{k}}$ is not much larger than $\Delta_{\mathbf{k}}$. In other words, in order to be observable in $N(\omega)$, the structure has to appear at a distance of at most $\delta k \sim \Delta/v_F$ from the Fermi line. At weak coupling this criterion is not satisfied and therefore Fig. 6 does not exhibit any deviations from the textbook form of the density of states for a d -wave superconductor.

We have solved the self-consistent equation Eq. (7) also for a larger interaction strength $U = 0.75W$, when the gap increases by more than an order of magnitude with respect to $U = W/2$. In this case we did find a nontrivial

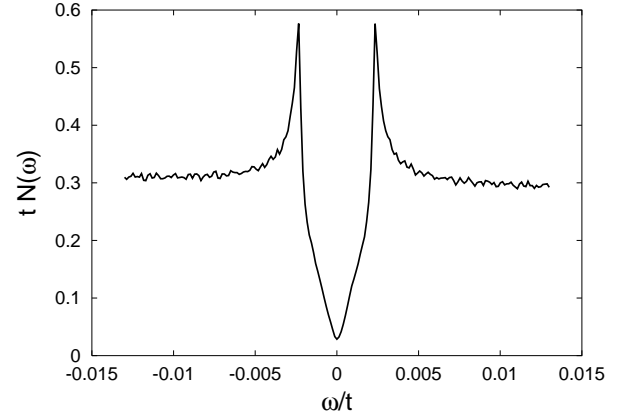


FIG. 6: Tunneling density of states for $U = W/2$, $t'/t = 0.3$, and $\rho = 0.8$. The superconducting gap obtained on a full lattice $L = 256 \times 256$ was linearly interpolated to a lattice $L = 8192 \times 8192$, over which the \mathbf{k} -summation in Eq. 9 is taken. The delta functions appearing in the electron spectral function Eq. 8 were given a finite width $\gamma/t = 1 \times 10^{-4}$.

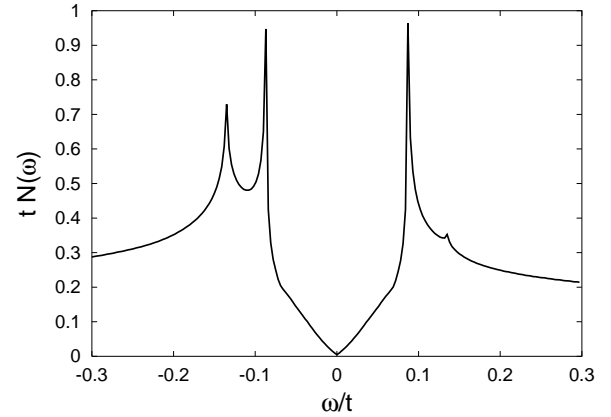


FIG. 7: Tunneling density of states for $U = 0.75W$, $t'/t = 0.3$, and $\rho = 0.8$. Calculated by the same method as in Fig. 6 with $\gamma/t = 5 \times 10^{-4}$.

structure in the density of states (see Fig. 7), which could however be attributed to the van Hove singularity in the density of states of the noninteracting spectrum rather than to a many body effect.

Now let us turn to the angular dependence of $\Delta_{\mathbf{k}}$. In Fig. 8 we plot $\Delta(\varphi)/\Delta(0)$ along the Fermi line for $T = 0$ and $T/t = 1$. The variable φ is the angle between the radius vector of the Fermi surface point under study [measured with respect to $M = (\pi, \pi)$] and the x axis. The overall shape of the high temperature data is close to the simple $\cos k_x - \cos k_y$ form of the gap. With decreasing temperature $\Delta_{\mathbf{k}}$ is seen to be locally more and more enhanced close to the crossing point of the Fermi line with the magnetic zone (hot spot). Nevertheless, this so-called hot spot effect is quite weak down to $T = 0$. Fig. 8 shows explicitly that the hot spot effect is in qualitative agreement with an earlier formulation⁹ in which

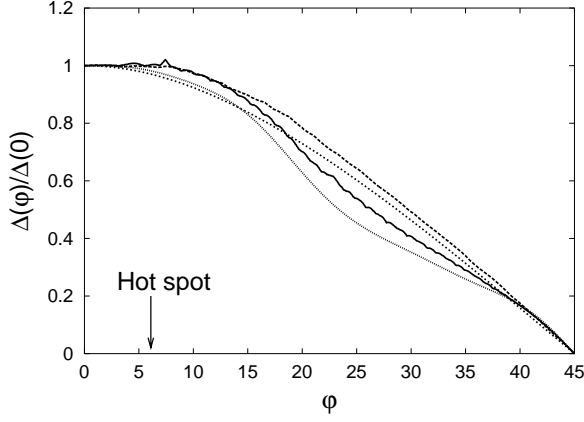


FIG. 8: Angular variation of a normalized superconducting gap along the Fermi line. Calculated on a full lattice $L = 256 \times 256$ for $U = W/2$, $t'/t = 0.3$, and $\rho = 0.8$. Top to bottom lines at $\varphi = 30^\circ$: $T/t = 1$, the simplest d -wave model function $\cos k_x - \cos k_y$, and $T = 0$; the lowest curve is a result obtained within the approach of Ref. 9.

the energy dependence of the Cooper channel interaction is neglected and $\Delta_{\mathbf{k}}$ lives only on the Fermi line. On the other hand, a recent paper¹⁹ reports (within the formalism of Ref. 9) a much stronger hot spot effect than found here.

IV. CONCLUSIONS

In conclusion, we have constructed a canonical transformation of the Hubbard model which eliminates quasi-particle scattering processes to first order in the interaction U . The resulting effective Hamiltonian contains terms of order U^2/W where W is the bandwidth, which are attractive in the Cooper channel. This allows us to construct a variational wavefunction for the Kohn-Luttinger superconductor and to show explicitly that even a purely repulsive model gains energy by developing superconducting correlations.

As an application of the method, the effective Hamiltonian has been solved in the BCS approximation and the superconducting phase diagram of the t - t' Hubbard model at half filling has been found. The superconduct-

ing state at $t'/t \sim 0.7$ is a weak-coupling analog of the wavefunction proposed for the J_1 - J_2 model by Capriotti *et al.*¹⁴

As another application, in the d -wave region of the t - t' Hubbard model⁹ we have found a nontrivial energy dependence of the gap function reminiscent of strong-coupling effects in conventional superconductors. There is a hot spot effect in the angular dependence of $\Delta_{\mathbf{k}}$, which is quite consistent with the estimates from calculations⁹ in which the gap lives only on the Fermi line.

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APPENDIX

As a test of the applicability of the variational method to an effective electronic Hamiltonian, we apply it to the case of phonon mediated superconductivity. We consider the simplest model of electrons with a local coupling to a phonon mode. The Hamiltonian of the system can be written $H = H_0 + H'$, where

$$H_0 = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \sum_{\mathbf{q} \neq 0} \omega_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}},$$

$$H' = \frac{D}{\sqrt{L}} \sum_{\mathbf{k}, \sigma, \mathbf{q} \neq 0} c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma} (a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger). \quad (\text{A.1})$$

Following Fröhlich,⁵ we seek a canonical transformation $\tilde{H} = e^{iS} H e^{-iS}$ which eliminates electron-phonon coupling to first order in D . This is accomplished by

$$iS = \frac{D}{\sqrt{L}} \sum_{\mathbf{k}, \sigma, \mathbf{q} \neq 0} \left(\frac{c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma} a_{\mathbf{q}}}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \omega_{\mathbf{q}}} + \frac{c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma} a_{-\mathbf{q}}^\dagger}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} + \omega_{\mathbf{q}}} \right), \quad (\text{A.2})$$

since, as one verifies easily, $[iS, H_0] = -H'$. The effective Hamiltonian can therefore be written as $\tilde{H} = H_0 + \tilde{H}'$ where, to second order in D ,

$$\tilde{H}' = \frac{1}{2} [iS, H'] = \frac{1}{L} \sum_{\mathbf{k}, \mathbf{k}', \sigma, \sigma'} \sum_{\mathbf{q} \neq 0} \frac{D^2 \omega_{\mathbf{q}}}{(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}})^2 - \omega_{\mathbf{q}}^2} c_{\mathbf{k}'-\mathbf{q}, \sigma'}^\dagger c_{\mathbf{k}', \sigma'} c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}, \sigma}$$

$$+ \frac{D^2}{2L} \sum_{\mathbf{q} \neq 0} \sum_{\mathbf{q}' \neq 0} \sum_{\mathbf{k}, \sigma} (c_{\mathbf{k}+\mathbf{q}, \sigma}^\dagger c_{\mathbf{k}-\mathbf{q}', \sigma} - c_{\mathbf{k}+\mathbf{q}+\mathbf{q}', \sigma}^\dagger c_{\mathbf{k}, \sigma}) \left[\frac{a_{\mathbf{q}}(a_{\mathbf{q}'} + a_{-\mathbf{q}'}^\dagger)}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \omega_{\mathbf{q}}} + \frac{a_{-\mathbf{q}'}^\dagger(a_{\mathbf{q}'} + a_{-\mathbf{q}'}^\dagger)}{\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}} - \omega_{\mathbf{q}}} \right].$$

The expectation value of \tilde{H}' in the product of a BCS state with a phonon state diagonalizing H_0 , $|\tilde{\psi}\rangle$, simplifies to

$$E = \langle \tilde{\psi} | \tilde{H}' | \tilde{\psi} \rangle = \frac{1}{L} \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}, \mathbf{k}'} b_{\mathbf{k}'}^* b_{\mathbf{k}} + \frac{D^2}{L} \sum_{\mathbf{k}, \mathbf{k}', \sigma} \frac{f_{\mathbf{k}\sigma}(1 - f_{\mathbf{k}'\sigma})}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} - \omega_{\mathbf{k}-\mathbf{k}'}} + \sum_{\mathbf{q} \neq 0} \delta\omega_{\mathbf{q}} n(\omega_{\mathbf{q}}),$$

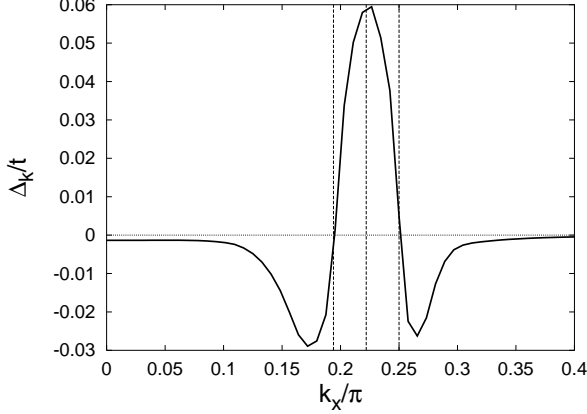


FIG. 9: Cut of the superconducting gap for phonon mediated superconductivity along the line $k_y = \pi$. Calculated on a full lattice $L = 256 \times 256$ for $t'/t = 0.45$, and $\rho = 1.0$. The phonon parameters are $\omega_0/t = 0.2$ and $\Gamma/t = 0.02$ and the electron-phonon coupling $D/t = 0.51$. The dashed vertical lines correspond to quasiparticle energies $\xi_{\mathbf{k}} = 0$ and $\pm\omega_0$.

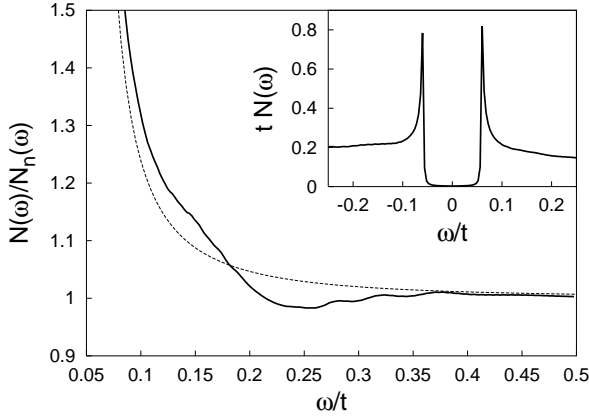


FIG. 10: Density of states in the superconducting state $N(\omega)$ normalized by its value in the normal state $N_n(\omega)$. Calculated from the data in Fig. 9 making use of the same method as in Fig. 6. The dashed line is the BCS approximation $N(\omega)/N_n(\omega) = \omega/\sqrt{\omega^2 - \Delta^2}$ with $\Delta = 0.059t$.

where $n(\omega)$ is the Bose distribution function. The first term describes the effective phonon mediated electron-electron interaction in the Cooper channel with $V_{\mathbf{k}, \mathbf{k}'} = 2D^2\omega_{\mathbf{k}-\mathbf{k}'}/[(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} - \omega_{\mathbf{k}-\mathbf{k}'})^2 - \omega_{\mathbf{k}-\mathbf{k}'}^2]$, the second term is the standard second-order perturbation theory correction to the ground state energy of the electron system, and the last term with $\delta\omega_{\mathbf{q}} = -2D^2\chi_1(\mathbf{q}, \omega_{\mathbf{q}})$ is the phonon energy renormalization.

In order to facilitate a numerical solution of the gap equation Eq. (7) for phonon mediated pairing, we have made use of a Cooper channel interaction

$$V_{\mathbf{k}, \mathbf{k}'} = D^2 \text{Re} \sum_{\sigma=\pm} \frac{\sigma}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} + \sigma(\omega_{\mathbf{k}-\mathbf{k}'} + i\Gamma)},$$

regularized by a finite phonon lifetime Γ . The BCS gap equation has been solved numerically on the same t - t' square lattice as for the Hubbard model. The superconducting gap obtained numerically for an Einstein mode with frequency $\omega_0/t = 0.2$ and $\Gamma/t = 0.02$ for electronic parameters $t'/t = 0.45$ and $\rho = 1.0$ and electron-phonon coupling $D/t = 0.51$ is shown in Fig. 9. Note that the gap changes sign in the vicinity of the phonon energy ω_0 . This nontrivial energy dependence of $\Delta_{\mathbf{k}}$ translates into a feature of the tunneling density of states in the same energy region, see Fig. 10. It should be pointed out that although both of the above results are in qualitative agreement with the Eliashberg theory,²⁰ there is one important difference of the present approach with respect to Ref. 20. Namely, within the Eliashberg theory the features of $\Delta(\omega)$ and $N(\omega)$ occur at energy $\omega_0 + \Delta(0)$ and not ω_0 as in our case. This difference is presumably due to the fact that within the canonical transformation approach, it is the bare electron energies which enter the energy denominators in Eq. (A.2) and not the renormalized energies as in the Eliashberg theory. However, in a truly weak coupling theory this difference is marginal.

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